Modeling the Response of Single Crystals to High-strain-rate Deformation

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The goal of this work is to formulate a constitutive model for the deformation of metallic single crystals over a wide range of strain rates, which is integral to computing reliable stress states of metallic polycrystals under shock loading. An elastic-viscoplastic, slip-based single-crystal model that accounts for crystallographic orientation, temperature, and strain-rate dependence has been formulated based on dislocation dynamics simulations and existing experimental data. Dislocation densities are separated according to type and given a systematic set of adaptable interaction rates. This allows the tracking of each dislocation event statistically. The direct use of dislocation density as a state variable also gives a measurable physical mechanism to strain hardening. The plastic model transitions from the low-rate, thermally activated regime to the high-rate, drag-dominated regime by use of a distribution of dislocation velocities, including kinetic effects. The model has been compared favorably with copper. The novelty of this model is that, for the first time, transition to drag-dominated dislocation motion is predicted rather than empirically fit to experimental data.

This document reports progress on a model for deformation of a single-crystal volume at a variety of strain rates from quasi-static to shock-loading. It includes temperature and pressure effects and the ability for improved validation information using dislocation densities. The end goal is to embed this single-crystal material model into a framework for simulating polycrystalline materials (such as finite element) in order to probe the variation in stress states caused by the microstructural differences. Information about these stress states leads to information about potential damage sites, which can be incorporated into the polycrystalline configuration to understand damage progression and improve modeling capabilities by incorporating salient features of the polycrystalline material.

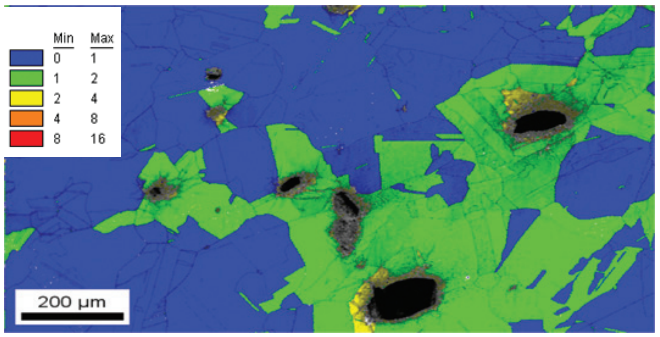

Fig. 1. Variation in single-crystal plastic behavior as evidenced by the average kernal misorientation in an electron back-scatter diffraction (ESBD) scan of copper that has been shocked for incipient damage. Scale is in degrees misorientation.

Understanding the response of single crystals to high-strain rate deformation provides the pathway to predicting microstructural effects in shocked polycrystals (see Fig. 1). Such effects are required to determine grain boundary stress states, which are the dominant factor in void nucleation for pure materials.

While the dislocation interactions themselves are being modeled for the single-crystal in this work, for tractability it is desired to have a statistical average over the dislocation interactions. Resolution of the individual dislocations is computationally too intensive, but the average reactions that take place in a section of material may be modeled to provide a more physical representation of the deformation process. It is also noted that to continue to higher strain rates, the motion of dislocations is believed to become drag-limited rather than thermally activated, requiring a transition in the average dislocation mechanics with strain-rate changes.

While many models exist which use dislocations as a state variable, none appear to consider the distribution of dislocation velocities. The dislocation density work of Wang, Beyerlein, and Lesar [1] showed that a small portion of the dislocations moved at a high velocity, causing the majority of the plastic deformation, while most dislocations moved at a lower velocity. This motivated the idea of using a distribution of dislocation velocities to model plastic deformation.

The plastic deformation evolution is based on statistical dislocation populations and the evolution of those populations. The material point volume is selected to be sufficiently large so that dislocation populations can be adequately described by a line density. Three main dislocation populations are considered: 1) glissile dislocations, which are free to move (ρ^M); 2) glissile dislocations, which currently do not move due to being blocked by obstacles–these are referred to as "pile up" (ρ^P), and 3) sessile dislocations acting as debris in the material (ρ^D). Mobile

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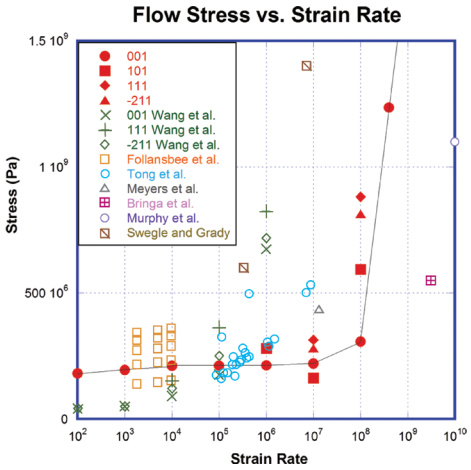

Fig. 2. Comparison of simulated flow stress at various strain rates to a variety of experimental Hopkinson bar, plate shock driven, laser driven, molecular dynamics, and dislocation dynamics simulations. Data taken from Wang, Beyerlein, and Lesar [2] and Armstrong and Zerilli [3].

dislocations (ρ^M) move through the crystal and are either blocked by obstacles, react and annihilate, react and become sessile, or exit the region. The population $\rho\{^P\}$ is distinguished as glissile, but is temporarily rendered immobile because it is stopped by other dislocations, substructure, or other impediments to dislocation glide, such as grain boundaries or inclusions. Pile-up dislocations can become mobile, react and annihilate, or react and become sessile. The population of dislocations ρ^D contains dislocations that are sessile and do not contribute to plastic strain–they are permanently immobile and are restricted to short thermal migratory motion. These sessile dislocations can be statistically stored or in an organized substructure. Statistically stored dislocations are randomly distributed. Substructure dislocations are concentrated in planar volumes.

The separation of dislocations into the mobile and pile-up populations is motivated by the dislocation dynamics work of Wang, Beyerlein, and LeSar, which concluded that a few elite dislocations carry the bulk of plastic deformation, where most dislocations have a comparatively low velocity. The motivation to model the distribution of dislocation velocities is used to create the simplest distribution of two populations moving at two velocities. Again for simplicity, one of the velocities is assumed to be insignificant and is approximated as zero. This differs from most current dislocation-based rate-sensitive plasticity models, which assume the entire dislocation population moves at the same velocity.

With parameters set to physical order of magnitude, the results of single-crystal tensile tests at various rates are compared to experimental copper tests. Results are seen in Fig. 2 for a single strain rate showing the prediction of the uniaxial stress state and dislocation density. Figure 3 shows that simulations predict an appropriate transition from thermally activated to drag-dominated dislocation motion, given the level of uncertainty in experimental data.

The key findings of this work to date are: 1) expansion of current direct simulation of polycrystals to include a single-crystal model capable of transitioning from low to high strain rates, and 2) prediction of the transition from thermally activated to drag-dominated strain rates. Further investigation is easily adaptable in the model. The model, when coupled with virtual polycrystal representations, allows for prediction of grain-boundary stress during shock experiments for determination of critical microstructure characteristics for damage.

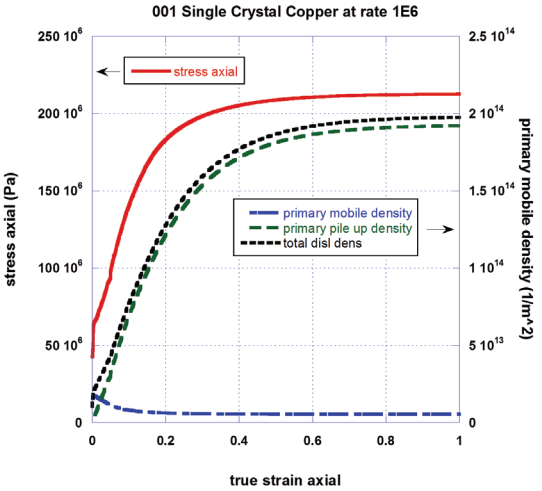

Fig. 3. Simulations of single crystals under tensile stresses using physically realistic parameters for copper were conducted to implement and validate the single-crystal model.

[1] Wang, Z.Q. et al., *Phil Mag* **87,** 2263 (2007).
[2] Wang, Z.Q. et al., *Int J Plast* **25,** 26 (2009).
[3] Armstrong, R.W. and F.J. Zerilli, *J Phys Appl Phys* **43,** 492002 (2010).

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